

Analysis of oxygen spectral lines in the 1.27 micron band for the ASCENDS mission

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Abstract— The ASCENDS mission requires simultaneous laser remote sensing of CO₂ and O₂ in order to convert CO₂ column number densities to average column CO₂ mixing ratios (XCO₂). As such, the CO₂ column number density and the O₂ column number density will be utilized to derive the average XCO₂ column. NASA Langley Research Center, working with its partners, is developing O₂ lidar technology in the 1.26-1.27- μ m band for surface pressure measurements. The O₂ model optical depth calculation is very sensitive to knowledge of the transmitted wavelengths and to the choice of Voigt input parameters. Modeling using the HITRAN database is being carried out to establish the evolution of candidate O₂ absorption lines as a function of atmospheric parameters such as altitude, temperature, and pressure. Preliminary results indicate limitations of the Voigt profile and the need to utilize more advanced models which take into account line mixing, line narrowing, and speed dependence. In this paper, we evaluate alternative lineshape models to establish the optimum lineshapes which better account for the variability of individual O₂ absorption lines at various atmospheric conditions. The combination of our modeling efforts with accurate laboratory measurements is anticipated to aid in achieving the desired CO₂ mixing ratio measurement accuracy requirement of for the ASCENDS mission.

Keywords—ASCENDS; Oxygen Lidar; CO₂ Mixing ratio; HITRAN; Voigt Profiles

I. INTRODUCTION

The National Research Council's (NRC) Decadal Survey (DS) of Earth Science and Applications from Space has identified the Active Sensing of CO₂ Emissions over Nights, Days, and Seasons (ASCENDS) as an important atmospheric science mission. The CO₂ mixing ratio needs to be measured to a precision of 0.5 percent of background or better (slightly less than 2 ppm) at 100-km horizontal resolution overland and 200-km resolution over oceans. To meet this goal, the ASCENDS mission requires simultaneous laser remote sensing of CO₂ and O₂ in order to convert CO₂ column number densities to average column CO₂ mixing ratios (XCO₂). As such, the CO₂ column number density and the O₂ column number density will be used to derive the average XCO₂

column. NASA Langley Research Center, working with its partners, is developing CO₂ and O₂ lidar technology in the 1.57- μ m and 1.26-1.27- μ m bands to be used for XCO₂ measurements.

In this paper we describe our ongoing modeling work and an improved modeling approach to enhance the accuracy of CO₂ and O₂ line-by-line transmission simulations. In particular, alternative lineshape models are evaluated to establish the optimum lineshapes which better account for the variability of individual absorption lines at various atmospheric conditions. In addition we are enhancing our models by incorporating new additional data such as the collision induced absorption cross-sections for the O₂ molecule and updated atmospheric profile models.

II. CO₂ AND O₂ TRANSMISSION MODELING

Our current CO₂ and O₂ transmission modeling efforts include the selection of the optimum laser wavelengths in the 1.57 and 1.26-1.27 micron bands by investigating the behavior of absorption lines in these bands as a function of altitude.

Traditional transmission simulation approach is based on the use of the HITRAN database [1] and as such has some accuracy limitations. Currently, the HITRAN database does not provide parameters required for modeling of spectral line shapes more accurate than Voigt. To achieve the accuracy set forth for the ASCENDS mission, the use of more sophisticated line shape models and consequently knowledge of additional spectral parameters unavailable in HITRAN is required. Several groups have done extensive measurements for the CO₂ molecule bands near 1.57 micron which provide more accurate and complete data than that currently available in the HITRAN database. For example, the recent studies by Devi et al. and Predoi-Cross et al provide additional data for line-by-line simulations such as pressure shift temperature dependence and speed dependent Voigt coefficients, as well as line-mixing parameters [2,3]. We used their results for line-by-line transmission modeling in the CO₂ band near 6348 cm⁻¹ as a replacement of the HITRAN database parameters to improve the accuracy of our CO₂ transmission calculations. For example, Fig 1 presents a comparison of the calculations carried out using HITRAN 2008 and the Devi & Predoi-Cross

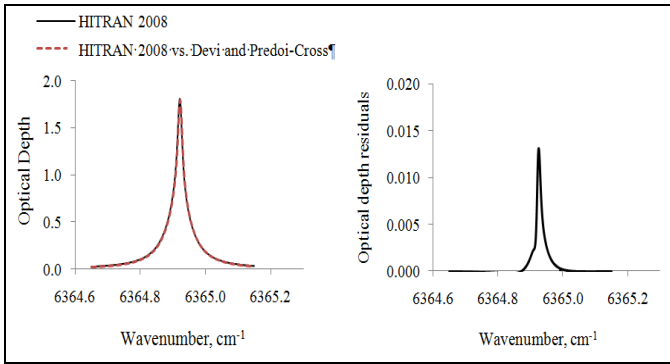


Figure 1. Comparison of calculations for a single CO₂ line near 6364.92 cm⁻¹ using the HITRAN 2008 [1] and Devi & Predoi-Cross data [2, 3].

data (Voigt profile; no speed dependence, line mixing or temperature dependence of line shifts is included). As can be seen, the differences in the spectral parameters alone result in residuals exceeding the required accuracy set forth for the ASCENDS mission measurements.

III. SUMMARY AND CONCLUSIONS

A summary of our modeling method is presented in Fig. 2. As can be seen, we are using previously reported data for speed dependent Voigt line-by-line transmission modeling of CO₂ atmospheric transmission. An extension of this approach onto the O₂ line-by-line simulations is planned after the required spectral parameters have been determined through experiments and least squares multispectral fitting. In addition, we are looking into supplementing our O₂ line-by-line transmission simulations with collision induced absorption data soon to be included in the HITRAN database (from: Dennis K. Killinger, Laurence S. Rothman, private communication).

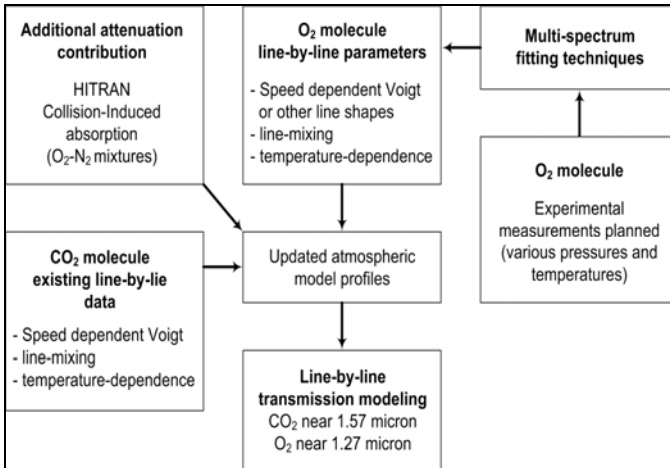


Figure 2. Summary of the modeling approach being implemented for the atmospheric transmission modeling of CO₂ and O₂.

Toward this end we have carried out preliminary simulation studies for the optimum selection of laser wavelengths for CO₂ and O₂ sensing. Our current work includes modification of our calculations by including the latest data. A speed dependent Voigt line-by-line modeling approach based on the latest data is being implemented to provide improved accuracy of CO₂ transmission calculations. Laboratory measurements are planned to obtain the required spectral parameters for O₂ line-by-line transmission calculations using more advanced lineshape models. The results of our calculations for selected CO₂ and O₂ lines at different atmospheric conditions will be presented.

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